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# A plausible explanation of non-zero isotope shifts in superconductors

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**Abstract** We propose to consider a charge Bose liquid model as a phenomenological explanation of three puzzling features of non-zero isotope shifts ($\alpha$) in superconductors These features are (i) large value of $\alpha$ 0 5) in normal superconductors, (ii) an overall trend of lower values of $\alpha$ with increasing $T_c$ and (iii) a very striking feature of negative value of $\alpha$ (= – 0 013 in Bi 2 2 2 3 with $T_c$ = 108K) [6] in high $T_c$ superconductors This phenomenon of non-zero isotope shifts observed in high $T_c$ oxides are explained on the baiss of (bi) polaronic theory

**Keywords** Isotope-shift exponent Polaron, nearest neighbour (*n n*) electron-phonon interaction (*e-ph*)

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## 1 Introduction

A charge Bose liquid, which was proposed by Schafrots [1] as a phenomenological explanation of superconductivity and later derived microscopically from Frohlich [2] electron-phonon (e-ph) interaction (bipolaronic superconductivity) is an intriguing possibility for high $T_c$ metal oxides From the research on superconductivity of strong electron-phonon (e-ph) interacting systems, we know that, the strong-coupling between electrons located at lattice sites with phonons leading to the generation of polarons/ bipolarons [3].

We propose to explain the phenomenon on the basis of small polaronic theory and suggest several plausible explanations. As for the apex oxygen anharmonicity, it is due to the polaronic effects as demonstrated by some works [4]. We propose to make an attempt in this direction to explain the observation of non-zero and negative $\alpha$ on the basis of small polaronic cloud. It is argued that some of these striking variation in $\alpha$ do not necessarily imply a large phonon contribution to $T_c$ and do not invalidate the electronic mechanism with a small phonon contribution Moreover, in BCS theory, there is no reason

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why $\alpha$ can not be negative, when the coulomb pseudo potential $\mu$ is comparable with the electron-phonon coupling constant

## 2. The model

In this work, we consider a single band Hubbard Model in the presence of a strong local (on-site) electron-phonon interaction Thus we start with the model Hamiltonian,

$$H = H_{hub} + H_{e\ ph} + H_{ph} \tag{1}$$

where $H_{hub}$ is the one band Hubbard Hamiltonian and is given by

$$H_{hub} \quad -\sum_{i\,j\,\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U\sum n_{i\uparrow} n_{i\downarrow} - \mu \sum n_{i\sigma} \tag{2}$$

where $t_{ij}$ denotes the hopping energy of an electron between the lattice sites $i$ and $j$ $c^{+}_{i\sigma}\,(c_{i\sigma})$ represents the electron creation (annihilation) operator of spin $\sigma(-\pm 1$ for both up and down spins, respectively) at lattice site $i$, $n_{i\sigma} + c^{+}_{i\sigma} c_{j\sigma}$ is the number operator U is the on-site Hubbard interaction term $\mu$ is the chemical potential introduced due to doping

$H_{e-ph}$ is the on-site electron-phonon term,

$$H_{e-ph} = \sum g_i(q)\left(b_q + b^{+}_{-q}\right) \tag{3}$$

Here $g_i(q)$ is the strength of the on-site electron-phonon interaction term and is expressed by,

$$g_i(q) = \sum_{2NM_1w_1} \left\langle \frac{\partial V}{\partial R_1}\, i \right\rangle \exp\left(-i\boldsymbol{q}\,\boldsymbol{R}_1\right) \tag{4}$$

Also $H_{ph}$ is the free phonon term in eqn (1)

$$H_{ph} = \sum \omega_q b^{+}_q b_q \tag{5}$$

Now we will perform a canonical transformation exp($S$) $H$ exp ($-S$) with respect to the local *e–ph* interaction generated through the operator,

$$S = \sum_q \frac{g_i(q)}{\omega_q}\left(b^{+}_q - b_{-q}\right). \tag{6}$$

Thus one eliminates the term $H_{e\text{-}ph}$ from the resulting Hamiltonian $H$ for narrow band system Thus one obtains the Hamiltonian, having the site energies renormalised and

also repulsive on-site interaction reduced by the polaronic self-energy Thus, the model polaronic Hamiltonian for narrow band system is obtained as,

$$H = -t_p \sum_{i,j\sigma} c^{+}_{i\sigma} c_{j\sigma} + U_e \sum_{i} n_{i\uparrow} n_{i\downarrow} - V \sum_{ij} n_i\, n_j - \sum_{i} \mu\, n_i \,. \tag{7}$$

This Hamiltonian is just like the Hamiltonian [5] with only an extra term of $\mu$, chemical potential where $t_p = t \exp(-g^2)$ is the polaronic hopping, $t$ is the bare hopping and $g$ denotes the electron-phonon (e-ph) coupling strength The effective on-site Coulomb repulsion is $U_e$ given by,

$$U_e = U - 2E_p,$$

where $$E_p = \sum' \frac{|g_i(q)|^2}{\quad} \tag{8}$$

$V$ in eq (7) is the inter-site attraction induced by the *e-ph* coupling

In strong-coupling narrow band systems, the Migdal theorem breaks down in the so-called anti-adiabatic limit [7], *i e*, when $\omega \geq W_p$, $\omega$ being the characteristic phonon freuency and $W_p$ is a renormalised half-bandwidth.

For moderate values of $g$, $W_p \geq V$, the small polarons form spatially overlapping Copper pairs, the regime of BCS-type polaronic superconductivity For large values of $g$, $t_p$ is very small and for $W_p << V$, bipolarons may form

## 3 Calculation of $T_c$

Now the second and third terms on the right hand side of the eq (7) is simplified by Hartree-Fock approximation with introduction of the order parameters

$$\Delta_0 = \langle c_{i\downarrow} c_{i\uparrow} \rangle \tag{9}$$

$$\Delta_1 = \frac{1}{2}\left( \langle c_{i\downarrow} c_{j\uparrow} \rangle + \langle c_{j\downarrow} c_{i\uparrow} \rangle \right). \tag{10}$$

Then the Hamiltonian, in the BCS form, may be written as,

$$H = \sum_{k\sigma} \xi_k\, \eta_{k\sigma} + \sum \Delta_k \left( c^{+}_{k\uparrow}\, c^{+}_{-k\downarrow} + h.c \right) \tag{11}$$

where, $\xi_k = \epsilon_k - \mu$, $\epsilon_k = -t_p\, Z\gamma_k$ and $\gamma_k = 1/Z \sum_{ij} \exp\left(i\mathbf{k}.\mathbf{R}_{ij}\right)$; $\mathbf{R}_{ij}$ being the nearest neighbour lattice vector. For a square lattice $\gamma_k = \cos kx + \cos ky$ and $Z = 4$ Then the

superconducting gap parameter is given by,

$$\Delta_k = U_e \Delta_0 - Z\gamma_k V \Delta_1 . \tag{12}$$

Now using the Green's function technique, the superconducting correlation is obtained as for BCS superconductors

$$\left\langle c^{+}_{k\uparrow}\, c^{\prime}_{-k\downarrow} \right\rangle = -\frac{\Delta_k}{2E_k} \tan h\left( \frac{\beta E_k}{2} \right) \tag{13}$$

where, $E_k = \sqrt{\xi_k^2 + \Delta^2}$ and $\beta = \frac{1}{k_\beta T}$.

Combining eqs (12) and (13) one obtains at $T = T_c$,

$$1 = ZVI_1\left( \frac{\Delta_1}{\Delta_0} \right) - U_e\, I_0 \tag{14}$$

and

$$1 = ZVI_2 - U_e\, I_1\left( \frac{\Delta_1}{\Delta_0} \right) \tag{15}$$

where

$$I_n = \int_1^{+1} d\epsilon_r .N(\epsilon_r). \frac{\epsilon_r^n}{2(\epsilon_r - \mu_r)} .\tan h\left( \beta_e^r \frac{\epsilon_r - \mu_r}{2} \right). \tag{16}$$

For, $n$ = 0, 1, 2,....

Where the subscript $r$ denotes a reduced variable expressed in units of the polaronic half band width $W_p = W_b \exp(-g^2)$, where $W_b$ ( = $zt$) is the half-bandwidth of the bare electronic band. Here $N(\epsilon_r)$ is the electron density of states.

Combining the set of coupled eqs (14) and (15) we get for $T_c$,

$$1 = ZV\left( I_2 - \frac{U_e I_1^2}{1 + U_e I_0} \right) \tag{17}$$

Following Alexandrov [7], the eq. (17) may be written as,

$$1 = ZVJ_2 + 2ZV\mu_r J_1 + \left( ZV\mu_r^2 - U_e \right) \cdot J_0 + ZVU_e \left( J_0 J_2 - J_1^2 \right) \tag{18}$$

where

$$J_n = \int_{-1}^{1} d\epsilon_r .N(\epsilon_r). \frac{1}{2}(\epsilon_r - \mu_r)^{n-1} \cdot \tan h\left( \beta_c^r \frac{\epsilon_r - \mu_r}{2} \right) \tag{19}$$

with $n$ = 0, 1, 2.....

It should be noted that in the weak coupling limit the values of the integrals $J_1$ and $J_2$ are much smaller than $J_0$. Also in the weak coupling limit ($W_p >> ZV$) we assume, $J_1 = J = 0$ and then $J_0$ takes the form as

$$J_0 = \frac{1}{2W_n} \ln \left( 1.14 \beta_c^r \sqrt{1 - \mu_r^2} \right) \tag{20}$$

then we get the approximate expression for $T_c$ as,

$$T_r^{approx} - 1.14 W_p \sqrt{1 - \mu_r^2} \cdot \exp \left| \frac{2W_p}{ZV \mu_r^2 - U_e} \right. \tag{21}$$

## 4. Calculation of $\alpha$

The isotope-shift exponent ($\alpha$) is defined as,

$$\alpha = -(\partial \ln T_c / \partial \ln M). \tag{22}$$

Now, the factors which depend on the isotope mass (M) are as follows :

$$g^2 \propto \sqrt{M}, W_p \propto \exp \left( g^2 \right), \tag{23}$$

i.e., $$\frac{dW_p}{dM} \sim \frac{1}{2\sqrt{M}} \tag{24}$$

It indicates that $W_p$ decreases with increasing isotopic mass which has been supported by Guo-meng Zhao *et al* [8] and Bussmann-Holder *et al* [9].

Now to derive an expression for $\alpha$ we have to differentiate eq. (7) with respect to $M$. Thus,

$$\alpha = \frac{g^2}{2} \left( 1 - \frac{1}{\beta_c^r} \cdot \frac{I_2 - 2I \cdot I_1 + I^2 I_0}{S_2 - 2IS_1 + I^2 S_0} \right) \tag{25}$$

where, $$I = \frac{U_e I_1}{1 + U_e I_0} \tag{26}$$

and $$S_n = \int_{-1}^{1} d\epsilon_r \cdot N(\epsilon_r) \cdot \frac{\epsilon_r^n}{4} \cdot \sec h^2 \left( \beta_c^r \frac{\epsilon_r - \mu_r}{2} \right. \tag{27}$$

with $n = 0, 1, 2$.

In the absence of effective coulomb repulsion ($U_c = 0$) the expression for $\alpha$ takes the form,

$$\alpha = \frac{g^2}{2}\left(1 - \frac{1}{ZV\beta_c^r S_2}\right). \tag{28}$$

The expression for $\alpha$ corresponding to $T_c^{approx}$ eq. (21) is

$$\alpha^{approx} = \frac{g^2}{2}\left(1 - \frac{2W_p}{ZV\,\mu_r^2 - U_e}\right) \tag{29}$$

## 5. Results and discussion

We have studied $T_c$ and $\alpha$ within the framework of a polaronic model as a function of the electron-phonon interaction strength ($g^2$) and doping (through chemical potential $\mu_r$) We also compared the results obtained from the approximated formulas (21) and (29). Naturally a suitable choice of parameters like $V$, $W_b$, $\mu_r$, $W_p$ are essential. Our choice of parameters is guided by the references [8] and [10].

In Figure 1 we have compared the variation of $T_c$ with $g^2$ from the exact and approximate eqs, in the absence of on-site repulsion, for two values of $\mu_r$ (0.6 and 0.4). $T_c$ obtained from the exact calculations increases with increasing $g^2$ *i.e.,* with decreasing polaronic bandwidth, and saturates to a value of V/3, independent of $\mu_r$, for large values of $g^2$.

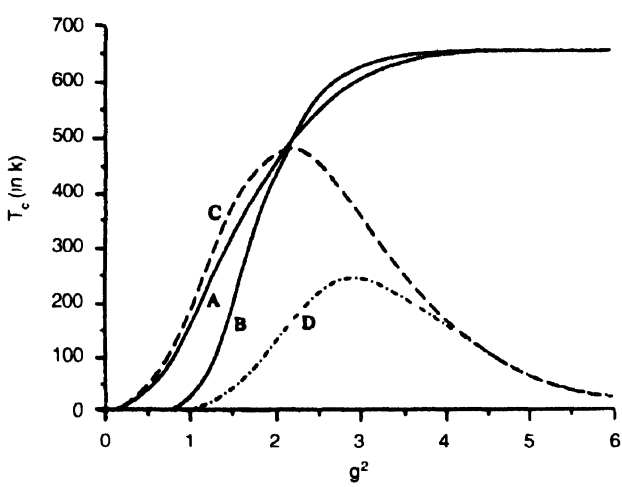


**Figure 1.** Variation of $T_c$ with $g^2$ for $V$ = 2000 $K$, $W_b$ = 12000 $K$ and $V_e$ = 0. For Curves A and C, $\mu_r$ = 0.6 and for Curves B and D, $\mu_r$ = 0.4. Solid curves are for exact value of $T_c$ and dotted $C$ curves are for approximate $T_c$.

In Figure 2 the variation of exact values of $\alpha$ (obtained from eq. 28) with $g^2$ is shown for $\mu_r$ = 0.6 and 0.4 $\alpha$ is negative for the entire range of $g$ values and becomes zero as

$g \to 0$ as well as for large values of $g$ where $T_c$ saturates, *i.e.*, $dT_c/dg^2 = 0$. For intermediate values of $g$, the region of interest for polaronic superconductivity, $\alpha$ is negative and decreases (becoming more negative) with decreasing values of $\mu_r$. For BCS-type polaronic superconductivity $\alpha$ is negative even for large $g$.

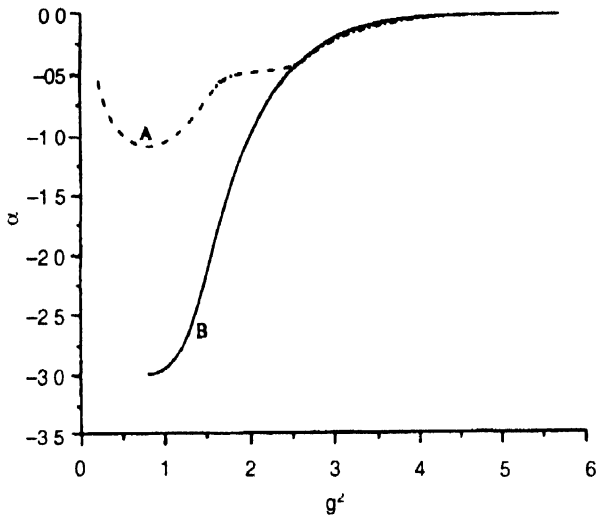


**Figure 2** Variation of exact $\alpha$ with $g^2$ for $W_b$ = 12000K and $V$ = 2000K. Curves *A* and *B* are for $\mu_r$ = 0 and 0.4. $U_c$ = 0 for all curves.

## 6. Conclusion

Our study shows that $\alpha$ is negative for polaronic BCS-type superconductivity for the entire range of doping and become more negative with the introduction of Coulomb repulsion. Positive values of $\alpha$ may be obtained within the polaronic theory for large values of $g$, where superconductivity is due to the Bose condensation of biopolarons.

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